Suppression of spin-orbit effects in 1D system

M.V. Entin and L.I. Magarill
Institute of Semiconductor Physics,
Siberian Branch of Russian Academy of Sciences
- 13 Lavrent'eva, Novosibirsk, 630090, Russia

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Abstract

We report the absence of spin effects such as spin-galvanic effect, spin polarization and spin current under static electric field and inter-spin-subband absorption in 1D system with spin-orbit interaction of arbitrary form. It was also shown that the accounting for the direct interaction of electron spin with magnetic field violates this statement.

The spin-orbit (SO) interaction in a 2D system underlies various spin control methods owing to the coupling between translational and spin degrees of freedom. Such effects have been studied as spin-galvanic effect [1]-[3], spin polarization [4]-[7] and spin current [8] under static electric field, spin polarization under action of electromagnetic wave [9]. The one dimensional system seems to be more suitable for this purpose due to more strong correlation between the spin and the wire direction. This stimulates to examine the similar problems in 1D systems.

We consider the 1D Hamiltonian

$$\mathcal{H} = \frac{p^2}{2m} + V(x) + \mathcal{H}_{SO} \tag{1}$$

with the most general form of SO interaction

$$\mathcal{H}_{SO} = \{(\mathbf{a}(x)\boldsymbol{\sigma}), p\}, \tag{2}$$

where $\boldsymbol{\sigma}$ are the Pauli matrices, the figure brackets denote the symmetrization procedure, vector $\mathbf{a}(x)$ is an arbitrary function of coordinate x along the wire. The Hamiltonian (2) originates from different approaches related with SO interaction in 1D systems. In general, it does not conserve the spin and hence one can expect the above mentioned effects in the frameworks of this Hamiltonian. However, we have found that in a strictly 1D system with the SO Hamiltonian (2) these effects vanish.

One-dimensional systems obeying the Hamiltonian (1-2)

For example, let us consider the 1D quantization of the 2D Rashba Hamiltonian [10],[11]

$$\hat{\mathcal{H}}_{SO} = \alpha_R(\boldsymbol{\sigma}[\mathbf{p} \times \mathbf{n}]), \tag{3}$$

where $\mathbf{p}$ is the 2D electron momentum, and $\mathbf{n}$ is the normal to the plane of the system (axis z). The size quantization in y direction leads to the reduction of the Hamiltonian (3) for the lowest subband:

$$\hat{\mathcal{H}}_{SO} = -\alpha_R \sigma_y p_x, \tag{4}$$

where $p_x = p$ is the 1D momentum. In this case the vector $\mathbf{a} = (0, -\alpha_R, 0)$.

The similar Hamiltonian arises in cubic crystals with no inversion symmetry from the spin-orbit term in the bulk Hamiltonian of Dresselhaus [12]

$$\hat{\mathcal{H}}^{(b)}_{SO} = (\delta_0/2)\varepsilon_{ijk}\sigma_i\lambda_{rsk}p_r p_j p_s,$$

where p_i is 3D electron momentum. The symmetric in all indexes tensor λ_{rsk} characterizes the anisotropy of the crystal. In the principal crystal axes λ_{rsk} has the only non-zero component $\lambda_{123} = 1$, in the general case $\lambda_{ijk} = \sum_{n\neq m\neq l} W_{in}W_{jm}W_{kl}$, where W_{ij} is the rotation matrix from the frame of reference of crystallographic axes to the laboratory system. The confinement along two directions, say y and z, converts $\hat{H}^{(b)}_{SO}$ into the 1D Hamiltonian, linear in the momentum p. The form of this Hamiltonian depends on the orientation of the wire relative to the principal crystal axes.

As the result of quantization we obtain

$$\mathbf{a} = \delta_0\Big(2\lambda_{xyz}(\overline{p_y^2} - \overline{p_z^2}),\ \ 2\lambda_{xxz}\overline{p_z^2} - \lambda_{zzz}\overline{p_z^2} - \lambda_{yyz}\overline{p_y^2},\ \ \lambda_{yyy}\overline{p_y^2} - 2\lambda_{yxx}\overline{p_y^2} + \lambda_{zzy}\overline{p_z^2}\Big), \tag{5}$$

where the overline means the averaging with the wave function of the ground state in quantum well.

In the considered cases the vector $\mathbf{a}$ is constant. More general is the situation of curved wire, in which the vector $\mathbf{a}$ becomes variable in accordance with the change of local direction of the axis x. The adiabatic Hamiltonian takes form of (1)-(2), where x is the coordinate along the wire, p is the conjugate momentum; the symmetrization reestablishes the hermicity.

The other factors of appearance of SO interaction in the form (2) are curvature-induced and torsion-induced SO interactions [13, 14]. In the particular case of a curved wire with axially symmetrical cross-section we have

$$\mathbf{a} = -\alpha A_{11}\kappa\mathbf{b}, \tag{6}$$

where $\mathbf{b}(x)$ denotes the binormal to the wire, $\kappa(x)$ is the curvature, α is the effective SO coupling constant of bulk crystal [13], $A_{11} = \langle(1 + 2q_1\partial_1)(\partial_1^2 + \partial_2^2))\rangle_0$ is the matrix element on the transversal wave function of the lowest subband of the wire. The quantity A_{11} has order of the energy of quantization in the wire.

Unitary transform

The SO Hamiltonian (2) is the most general local expression which has the first order in the SO constant and linear in p. The other form of the Hamiltonian (1) is

$$\mathcal{H} = \frac{m}{2}v^2 - \frac{a^2}{2} + V(x), \tag{7}$$

where the velocity operator is $v = p/m + (\mathbf{a}(x)\boldsymbol{\sigma})$. We shall demonstrate, that the Hamiltonian (7) can be unitary transformed to the form with no Pauli matrices. Let us consider an equation

$$(-i\frac{\partial}{\partial x} + (\mathbf{a}(x)\boldsymbol{\sigma}))U(x) = 0 \tag{8}$$

for an operator $U(x)$ which explicitly depends on the coordinate x. The solution of (8) is

$$U(x) = 1 + \sum_{n=1}(-i)^n \int_0^x dx_1 ... \int_0^{x_{n-1}} dx_n \ (\mathbf{a}(x_1)\boldsymbol{\sigma})...(\mathbf{a}(x_n)\boldsymbol{\sigma}). \tag{9}$$

The expression (9) can be rewritten as x-ordered exponent (similar to t-ordering with difference that the ordering should be done in x-space):

$$U(x) = T_x(\exp(-i\int_0^x dx(\mathbf{a}(x)\boldsymbol{\sigma}))) \equiv$$
$$\sum_n (-i)^n \frac{1}{n!}\int_0^x dx_1 ... \int_0^x dx_n T_x((\mathbf{a}(x_1)\boldsymbol{\sigma}))...(\mathbf{a}(x_n)\boldsymbol{\sigma}))). \tag{10}$$

The operation T_x means that all operators should be placed in the decreasing order of x_k. The inverse operator $U(x)^{-1}$ is determined by the ordering in the inverse order T_x^-:

$$U^{-1}(x) = T_x^-(\exp(+i\int_0^x dx(\mathbf{a}(x)\boldsymbol{\sigma}))). \tag{11}$$

The operator $U(x)$ is unitary: $U^+U = 1$; one can treat $U(x)$ as a spacial evolution operator. It can be expanded on the 2×2 matrix basis: $U = (1 + i(\mathbf{d}\boldsymbol{\sigma}))(1 + d^2)^{-1/2}$, where the real vector $\mathbf{d}$ satisfies an equation

$$\frac{\partial \mathbf{d}}{\partial x} + \mathbf{a} + (\mathbf{ad})\mathbf{d} - [\mathbf{ad}] = 0. \tag{12}$$

By means of the operator U the wave function transforms as $\psi(x) = U(x)\phi(x)$. The identities $vU(x)\phi(x) = U(x)(p/m)\phi(x)$ and $U(x)V(x) = V(x)U(x)$ are valid, that yields the transformation rules $U^+(x)vU(x) = p/m$ and $U^+(x)V(x)U(x) = V(x)$. The transformed spin operator $\boldsymbol{\sigma}(x) = U^+\boldsymbol{\sigma}U$ obeys the equation $\partial\boldsymbol{\sigma}(x)/\partial x = -2[\mathbf{a}\boldsymbol{\sigma}(x)]$ and has the explicit form $\boldsymbol{\sigma}(x) = (\boldsymbol{\sigma} + \mathbf{d}(\mathbf{d}\boldsymbol{\sigma}))/(1 + d^2)$.

Using these rules we find

$$\mathcal{H}' = U^{-1}\mathcal{H}U = \frac{p^2}{2m} + V(x) - \frac{a^2(x)}{2}. \tag{13}$$

Thus, the transformation excludes the spin from the Schrödinger equation. The Hamiltonian (13) immediately yields the spin degeneracy of electron states, unless the boundary conditions depend on spin explicitly. In particular, if the simple-connected wire is infinite in both direction and the states are localized, the boundary conditions $\psi \to 0$ yield $\phi \to 0$. This means double spin degeneracy (Kramers degeneracy). The delocalized states remain double-degenerate also.

Responses

The unitary transformation of the Hamiltonian to the form (13) has strong impact on different response functions. For example, consider linear responses of electric current $J = \sigma E$, spin polarization $S_i = \langle \sigma_i \rangle /2 = \gamma_i E$ and spin current $J_i^S = \langle \{\sigma_i, v\} \rangle /2 = \sigma_i^S E$. The electric field (tangent component) is assumed to be constant along the wire. These linear responses are expressed by the Kubo formula via the velocity or velocity-spin correlators

$$\frac{e}{L} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon d\epsilon' \frac{f(\epsilon') - f(\epsilon)}{\epsilon' - \epsilon} \frac{i}{\epsilon' - \epsilon + i\delta} \mathrm{Tr} \left(\delta(\epsilon - \mathcal{H}) v \delta(\epsilon' - \mathcal{H}) \mathcal{A}_i \right), \tag{14}$$

where in the case of conductivity $\mathcal{A}_i$ stands for the velocity operator v, for the spin orientation and spin current $\mathcal{A}_i = \sigma_i/2$ and $\mathcal{A}_i = \{v, \sigma_i\}/2$, respectively, $f(\epsilon)$ is the Fermi function, L is the length of the system.

More general expressions for responses in arbitrary order on the electric field are determined by the velocity correlators

$$\mathrm{Tr}(v\delta(\epsilon_1 - \mathcal{H}) v \delta(\epsilon_2 - \mathcal{H}) ... v \delta(\epsilon_3 - \mathcal{H})) \tag{15}$$

or spin-velocity correlators

$$\mathrm{Tr}(v\delta(\epsilon_1 - \mathcal{H}) v \delta(\epsilon_2 - \mathcal{H}) ... \sigma_i \delta(\epsilon_3 - \mathcal{H})). \tag{16}$$

Instead of the spin operator one can write the spin current operator $\{\sigma_i, v\}/2$.

Let us unitary transform operators inside the trace operation using transformation $A \to U^{-1} A U$. After the transformation the expression under Tr in (15) becomes unit in the spin space. The expression (15) reduces to

$$\mathrm{Tr}((p/m)\delta(\epsilon_1 - \mathcal{H}')(p/m)\delta(\epsilon_2 - \mathcal{H}') ... (p/m)\delta(\epsilon_3 - \mathcal{H}')) \tag{17}$$

and (16) goes to

$$\mathrm{Tr}((p/m)\delta(\epsilon_1 - \mathcal{H}')(p/m)\delta(\epsilon_2 - \mathcal{H}') ... \sigma_i(x)\delta(\epsilon_3 - \mathcal{H}')) = 0. \tag{18}$$

As a result of (17), the conductivity of the system with SO interaction converts to that of the system with no SO interaction. The eq.(18) follows from the identity $\mathrm{Tr}_\sigma(\boldsymbol{\sigma}(x)) \equiv 0$, where Tr_σ denotes the trace in the spin space. It proves that both coefficients of spin polarization γ_i and spin current σ_i^S vanish. Similar conclusions can be done with respect to electrical responses of higher orders (*e.g.*, the photogalvanic effect) which are not subjected to SO interaction and spin responses on the electric field (e.g., stationary spin orientation by alternating electric field) which vanish.

Note, that for proof of (18) it is essential the presence of *the only* spin operator under the trace; the similar correlators, containing two or more spin operators do not vanish. Note also, that the proof can be reformulated in the terms of the wave function. In fact, the wave function can be decomposed to the product of spinor function $\chi(x)$, obeying the equation $v\chi(x) = 0$ and scalar function $\phi(x)$ obeying the Schrödinger equation with the Hamiltonian (7). The separation of variables can be done for the Green functions: they decay on a product of the coordinate Green function $G_E(x, x')$ of the Hamiltonian (7) and spin functions $U(x)U^+(x')$.

Possible generalizations

In this section we consider possible generalizations of the Hamiltonian (7) which conserve the main conclusions. First, we can include the electric field into the potential $V(x)$, hence all conclusions remain valid in presence of it in any order of magnitude.

Second, we can consider the potential as periodic (or containing periodic part together with random one). Such potential without the SO interaction forms the energy bands $\epsilon(p)$, where p is now quasimomentum. The operator p/m in SO part goes to $\partial\epsilon/\partial p$. Hence the resulting new Hamiltonian can be also converted to the form with no spin operators.

Third, the spin can be treated as a quantum number, counting any pair-degenerate levels. For example, they can be subbands, originated from two equivalent valleys of bulk semiconductor. The Hamiltonian (1) in that case refers to the system with valley degeneracy without spin. According to the found transform, the valley degeneracy will not be lifted.

Fourth, we can include spin-independent e-e interaction. As such Hamiltonian does not touch the spin, the transformation can be done also.

What limits the spin elimination?

From said above one can conclude that there is no spin-orbit interaction in 1D system. In fact, this is not the case. The spin does not commute with the Hamiltonian (7). Hence, an electron with a preset spin, once injected into the wire, will change the spin during propagation along the wire.

In particular, this manifests itself in the systems with magnetic spin injectors/spin-selective drains [15], where the boundary conditions break the form of the Hamiltonian (7). (In the magnetic injector one should supplement the Hamiltonian with the exchange term like $J\boldsymbol{\sigma}\boldsymbol{\Xi}$, where $\boldsymbol{\Xi}$ is the mean spin density in the contact, J is the exchange constant). Conductance of a finite wire with spin-selective source and drain should be sensitive to the spin evolution caused by the SO interaction. Thus, the total system does not obey the conditions of the proof.

The same is valid for cyclic systems, *e.g.* a ring. The periodic boundary condition in the ring of length L, $\psi(L) = \psi(0)$ converts into the equation $U(L)\phi(L) = \phi(0)$, containing the spin via the operator U. Hence, the spin operator, being eliminated from the Schrödinger equation, appears in the boundary conditions that produces the spin splitting of levels.

We have neglected the Zeeman term in the Hamiltonian, direct interaction of spin with the magnetic field. This term actually leads to the spin-flip transitions caused by the alternating magnetic field and other effects. Due to relativistic smallness they are weak. An example of such effect is examined below.

Example: EPR-induced photogalvanic effect in spiral quantum wire

We consider here a spiral quantum wire with circular cross-section. In this system the alternating electromagnetic field can cause the steady electric current [16, 17]. We have previously studied the system neglecting the SO interaction. With taking into account SO interaction the possibility of resonant current caused by spin-flip processes arises. In

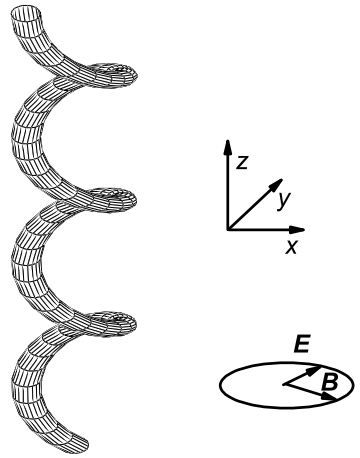

Figure 1: Spiral quantum wire.

accordance with said above, the *electric* component of field can not induce such current. Hence the direct interaction of spin with magnetic field (EPR-resonance) should be taken into account. The equation of central line of helical wire is

$$\mathbf{r} = (R\cos(kq), R\sin(kq), \eta q), \tag{19}$$

where R is the radius of the helix, q is the coordinate (length) along the helix, the pitch of the helix is $2\pi\sqrt{1/k^2 - R^2}$. The sign of k determines the helix direction $\xi = \pm 1$. The spiral symmetry of the wire with respect to translations along the wire ($q \to q + \Delta$) helps to find exact electron states. The adiabatic 1D Hamiltonian reads [14]

$$\frac{1}{2m}(p + \frac{e}{c}\mathbf{At})^2 - \alpha A_{11}\kappa\{(\mathbf{b}\boldsymbol{\sigma}), (p + \frac{e}{c}\mathbf{At})\} + V(q) + \frac{1}{2}g\mu_B\boldsymbol{\sigma}\mathbf{B}, \tag{20}$$

where $p = -i\partial_q$, $\mathbf{t}(q) = (-kR\sin(kq), kR\cos(kq), \eta)$ is the tangent ort to the wire, $\mathbf{b}(q) = (\eta\sin(kq), \eta\cos(kq), kR)$ is the binormal, $\mathbf{A}(t)$ is the vector-potential of electromagnetic wave polarized in x, y plane; the last (Zeemann) term describes interaction of spin with alternating magnetic field

$$\mathbf{B}(t) = (\mathbf{B_0}\exp(-i\omega t) + c.c.)/2.$$

Without the Zeemann term the spin can be excluded, as mentioned above and the problem is reduced to the spinless one [17]. The Zeemann term results in the photogalvanic effect caused by transitions between spin-splitted subbands.

Let us consider the magnetic field polarized in the plane (x, y). The wire symmetry imposes the current phenomenology of the form $J_{PG} \propto \xi[\mathbf{B}_0, \mathbf{B}_0^*]_z$. The contribution to the stationary current due to interaction of electron spin with magnetic field is given by the quadratic Kubo-type formula:

$$J_{PG} = \frac{e}{8L} g^2 \mu_B^2 \ \mathrm{Re}\Big\{ B_{0i} B_{0j}^* \int d\epsilon d\epsilon' d\epsilon'' \frac{f(\epsilon') - f(\epsilon'')}{\delta + i(\omega + \epsilon' - \epsilon'')} \times \Big[\frac{C_{ij}(\epsilon, \epsilon', \epsilon'')}{2\delta + i(\epsilon - \epsilon'')} - \frac{C_{ji}(\epsilon', \epsilon'', \epsilon)}{2\delta - i(\epsilon - \epsilon')} \Big] \Big\}, \tag{21}$$

where $C_{ij}(\epsilon, \epsilon', \epsilon'') = \mathrm{Tr}(v\delta(\epsilon - \mathcal{H}))\sigma_i \delta(\epsilon' - \mathcal{H}))\sigma_j \delta(\epsilon'' - \mathcal{H}))$ is the velocity-spin-spin correlator, $\mathcal{H}$ is the Hamiltonian (20) in the absence of external field ($\mathbf{A} = 0, \mathbf{B} = 0$). We shall neglect complications caused by the localization of electron states in 1D system and emulate the impurity scattering by the switching-on field: the rate of the field $\delta = 1/2\tau$ replaces the reciprocal relaxation time $1/\tau$.

The resulting current is

$$J_{PG} = \frac{1}{8} e\tau (g\mu_B)^2 \xi \ \mathrm{Im}[\mathbf{B}_0, \mathbf{B}_0^*]_z \left[f(\frac{2m\omega - C^2}{2C}) - f(\frac{2m\omega + C^2}{2C}) \right], \tag{22}$$

where

$$C = 2m\alpha A_{11} \frac{1}{R} R^2 |k|^3. \tag{23}$$

The current exists in a narrow window of frequencies corresponding to the permitted spin-flip transitions. When SO interaction is switched off the width of window (but not the current magnitude) shrinks.

Thus, the direct interaction of the spin with the magnetic field of the wave results in the spin-guided translational effect.

The EPR-induced photogalvanic effect should be compared with the photogalvanic effect caused by the action of electrical field on the translational motion of electron [17]; the latter exists in the absence of SO interaction. For a running electromagnetic wave both effects add together, for a standing wave (e.g., in resonator) they can be observed separately if to place the wire in loop or node of corresponding fields. Besides, they have different frequency dependencies.

In conclusion, we have found that in 1D systems different response function, which does not include the spin degree of freedom are not influenced by spin-orbit interaction. The responses connecting the spin and translational degrees of freedom are nonexistent unless the direct magnetic-field spin-flip processes are taken into account. On the contrary, the inclusion of such interaction leads to the magnetic-field-induced resonant steady current.

In contrast to 2D systems, where SO interaction plays determinative role for phenomena involving charge transfer and spin, in 1D systems the influence of SO interaction is suppressed. The transition from 2D to 1D due to lateral quantization results in the sequential decrease of SO-induced effects.

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